Enhancing Hit Identification in *Mycobacterium tuberculosis* Drug Discovery Using Dual-Event Bayesian Models

Sean Ekins[1, 2*], Robert C. Reynolds[3,4], Scott G. Franzblau[5,], Baojie Wan[5] , Joel S. Freundlich[6,7] and Barry A. Bunin[1]

[1]Collaborative Drug Discovery, 1633 Bayshore Highway, Suite 342, Burlingame, CA 94010, USA.

[2]Collaborations in Chemistry, 5616 Hilltop Needmore Road, Fuquay-Varina, NC 27526, USA.

[3]Southern Research Institute, 2000 Ninth Avenue South, Birmingham, AL 35205, USA.

[4]Current address: University of Alabama at Birmingham, College of Arts and Sciences, Department of Chemistry, 1530 3rd Avenue South, Birmingham, Alabama 35294-1240, USA.

[5] Institute for Tuberculosis Research, University of Illinois at Chicago, Chicago, IL 60607, USA.
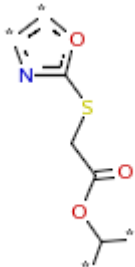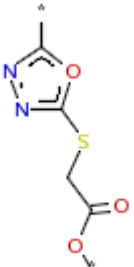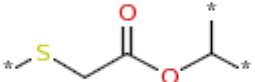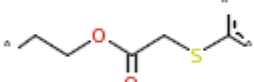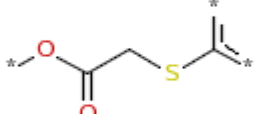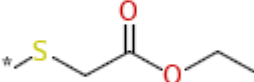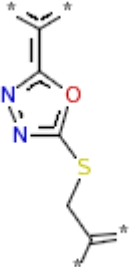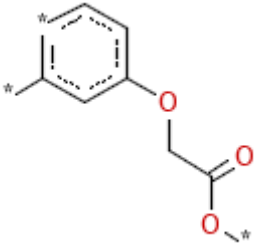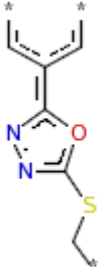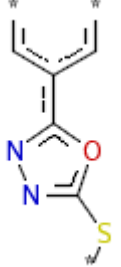
[6]Department of Medicine, Center for Emerging and Reemerging Pathogens, UMDNJ – New Jersey Medical School, 185 South Orange Avenue Newark, NJ 07103, USA.

[7]Department of Pharmacology & Physiology, UMDNJ – New Jersey Medical School, 185 South Orange Avenue Newark, NJ 07103, USA.

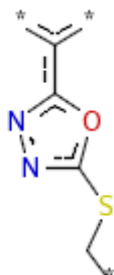*To whom correspondence should be addressed. (e-mail: ekinssean@yahoo.com)

Running Head: Dual Event Bayesian Models

Figure S1. MLSMR dose response and cytotoxicity model: good features from FCFP_6.

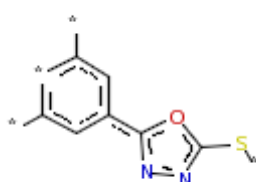|				
G1: -1449793464 21 out of 31 good Bayesian Score: 1.896	G2: -891643182 19 out of 27 good Bayesian Score: 1.895	G3: -60038150 49 out of 89 good Bayesian Score: 1.882	G4: 1670875748 24 out of 38 good Bayesian Score: 1.877	G5: 363977085 49 out of 92 good Bayesian Score: 1.853
G6: 854938188 21 out of 36 good Bayesian Score: 1.789	G7: -1387481105 25 out of 47 good Bayesian Score: 1.755	G8: 1209850658 12 out of 17 good Bayesian Score: 1.748	G9: -1700730929 24 out of 46 good Bayesian Score: 1.733	G10: 1476473713 24 out of 47 good Bayesian Score: 1.716
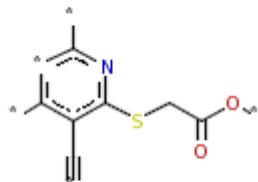
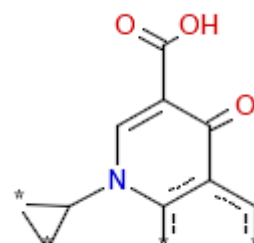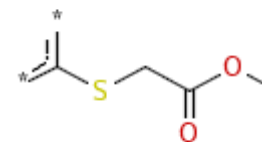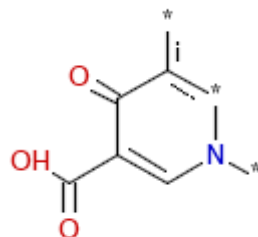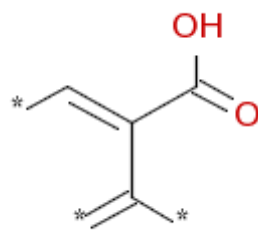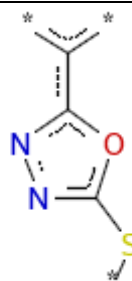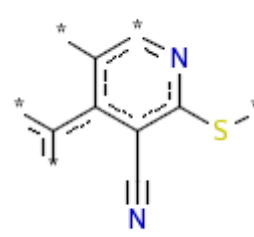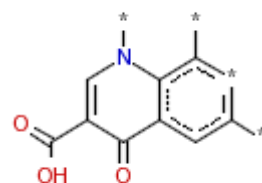|				
G11: -1943087851 9 out of 11 good Bayesian Score: 1.705	G12: 1941608633 25 out of 51 good Bayesian Score: 1.691	G13: -180488964 19 out of 37 good Bayesian Score: 1.674	G14: 1048446020 7 out of 7 good Bayesian Score: 1.660	G15: 1669687439 13 out of 23 good Bayesian Score: 1.642
G16: 173580544 8 out of 10 good Bayesian Score: 1.641	G17: 1393614142 8 out of 10 good Bayesian Score: 1.641	G18: -1048017265 25 out of 55 good Bayesian Score: 1.631	G19: 715653355 7 out of 8 good Bayesian Score: 1.613	G20: 192299924 7 out of 8 good Bayesian Score: 1.613